

6-Amino-4-hydroxynaphthalene-2-sulfonic acid
90-51-7 | DTXSID0026547

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 304 °C

Global applicability domain: Outside

Local applicability domain index: 1.28e-01

Confidence level: 5.01e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Trimellitic anhydride

Measured: 390

Predicted: 366

[Image not found](#)

Chloramben

Measured: 312

Predicted: 301

[Image not found](#)

Benzoic acid, 2-benzoyl-

Measured: 261

Predicted: 309

[Image not found](#)

Diphenylurea

Measured: 262

Predicted: 269